

A

**ZINC15 kinase subset**  
available now, anodyne

10883

**intersection with eMolecules library**

1204

**availability through eMolecules**

Tier1, 100 mg, powder

292

**predicted pKa filter**

Epik Sequential pKa

- at least one pKa value in range 3-11
- pKa values at least 1 pKa unit apart

180

**predicted logP filter**

$-1 \leq \text{OpenEye XlogP} \leq 6$

178

**FRAGMENT-LIKE**

**DRUG-LIKE**

$150 \leq \text{mw} < 350$

**molecular weight filter**

$350 < \text{mw} \leq 500$

126

47

**price listed and 100 mg available**

111

40

**filter out molecules with experimental logP**

91

15

**compound selection rules**

1. Include at least one molecule for each kinase inhibitor ring fragment
2. Limit the number of frequently appearing rings to at most one
3. Target broad and uniform sampling of logP dynamic range
4. Prioritize cheaper molecules

25 (17)

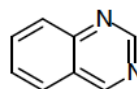
10 (7)

B

**Heterocycles found frequently in  
FDA approved kinase inhibitors**



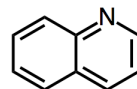
pyridine



quinazoline



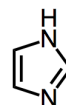
pyrimidine



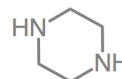
quinoline



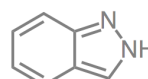
pyrrole



imidazole



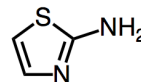
piperazine



indazole

C

**Heterocycles overrepresented in  
fragment libraries**



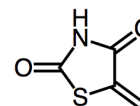
aminothiazole



thiophene



1,3,4-thiadiazole



5-methylenethiazolidine-2,4-dione